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Crossover Temperature from Non-Fermi Liquid to Fermi Liquid Behavior in Two Types of Impurity Kondo Model

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Numerical renormalization-group results on entropy of the anisotropic two-channel Kondo model with the band-width cutoff (D) in the presence of a magnetic field (h) are obtained to determine crossover temperature from the non-Fermi liquid to Fermi liquid fixed point. It is found that the crossover temperature ($T_{\rm x}$) is given by $T_{\rm x} \equiv rT_{\rm K} \sim D(\Delta J/J_{\rm av})^2 e^{-1/J_{\rm av}}$ when $(h/T_{\rm K})^2 \ll r \ll 1$, where $T_{\rm K}$, $J_{\rm av}$ and ΔJ are the Kondo temperature, the average and difference of the exchange coupling constants, respectively. This result indicates that non-Fermi liquid behavior can be seen even if $\Delta J > T_{\rm K}$. Robust similarities of the crossover behavior in the region around the non-Fermi liquid critical point to that of the two-impurity Kondo model are also discussed.

KEYWORDS: numerical renormalization-group method, two-channel Kondo model, two-impurity Kondo model, non-Fermil liquid

§1. Introduction

Non-Fermi-liquid (NFL) behavior observed in some heavy fermion compounds and High $T_{\rm c}$ cuprates has stimulated intense studies for a variety of impurity models which have NFL quantum-critical points.[1–5)] While each of the models has its own energy scale $T_{\rm K}$ below which the thermodynamic and transport properties are geverned by the NFL fixed point, relevant perturbation which is normaly present in real systems introduces another energy scale $T_{\rm x}$ where crossover to the Fermi-liquid (FL) fixed point occurs. In other words, the NFL behavior can be observed only when $T_{\rm x}/T_{\rm K} \ll 1$. Since real systems would not be exactly on the critical points, it is important to know about the above condition that NFL behavior occurs. In this paper, we investigate the crossover energy scale $T_{\rm x}$ so that the condition $T_{\rm x}/T_{\rm K} \ll 1$ is specified in a microscopic sense by using the

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numerical renormalization-group (NRG) method[6–8] for two types of the quantum impurity model, the two-channel Kondo model in the presence of a magnetic field and the two-impurity Kondo model, with a special emphasis on the effect of channel anisotropy.

The non-Fermi-liquid fixed point of the multichannel Kondo model in the overscreened case, i.e., when the number of channels n is larger than twice the size of impurity spin S, is characterized by a degeneracy of the ground state which cannot be completely lifted by coupling to conduction electrons.[1,9] The residual entropy is given by $\ln[\sin[(2S+1)\pi/(n+2)]/\sin[\pi/(n+2)]]$.[10,11] In temperature T below the Kondo temperature T_K, the specific heat coefficient γ and magnetic susceptivility χ are $\sim T^{4/(n+2)-1}$, the electrical resistivity ρ is $const. \pm T^{2/(n+2)}$.[10–13] A magnetic field or channel anisotropy is relevant so that it brings about crossover to Fermi-liquid fixed points but γ, χ and ρ keep the above scaling laws when $T_\mathrm{x} \ll T \ll T_\mathrm{K}$. Fig.1 presents a schematic phase diagram in the case of $n=2$, $S=1/2$ in which γ, $\chi \sim |\ln T|$ and $\rho \sim const. \pm \sqrt{T}$ in the region $T_\mathrm{x} \ll T \ll T_\mathrm{K}$. The two-channel Kondo model has been regarded as one of the most probable candidates responsible for the NFL behavior observed in U alloys.[2] Recently, the multichannel Kondo model with channel anisotropy has been discussed in relation to singular effects of impurities in the region around the ferromagnetic quantum-critical point.[14]

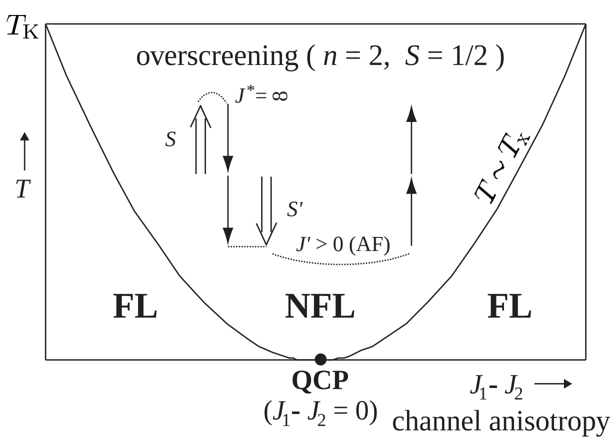

Fig. 1. A schematic phase diagram near a quantum-critical point (QCP) of the $n=2$, $S=1/2$ channel anisotropic Kondo model. In the region $T_\mathrm{x} \ll T \ll T_\mathrm{K}$, NFL behavior occurs due to the overscrening Kondo effect.

The crossover behavior to the FL fixed point in the $n=2$, $S=1/2$ Kondo model with channel anisotropy and/or in the presence of a magnetic field has been investigated by a variety of methods.[15–22] It can be easily seen in the impurity entropy which decreases from $\ln\sqrt{2}$ to 0 around T_x

as temperature is lowered. The crossover temperature $T_{\rm x}$ is proportional to the square of relevant perturbation as follows:

$$T_{\rm x} \propto h^2, \tag{1.1a}$$

in the presense of a magnetic field H where $h = \mu_{\rm B} H$;

$$T_{\rm x} \propto (J_1 - J_2)^2, \tag{1.1b}$$

in the channel anisotropic case where J_1 and J_2 are the exchange couplings for two channels, respectively.[16,17] On the other hand, the impurity free energy $F_{\rm imp}$ has the following scaling form:

$$F_{\rm imp}(r; T, h) = -T f(r, T/T_{\rm K}, h/T), \tag{1.2}$$

where r is a dimensionless function of D, J_1 and J_2 which depends on a cutoff scheme and in general unknown.[21] Since r represents channel anisotropy, $r = 0$ if $J_1 = J_2$. From eqs. (1.1a) and (1.2), we can easily see that $T_{\rm x} \sim h^2/T_{\rm K}$ so that crossover from NFL to FL regime occurs if $(h/T_{\rm K})^2 \ll 1$ in the isotropic channel case.[9,15,17] In the case of channel anisotropy, however, eqs. (1.1b) and (1.2) tell us nothing about the condition that the NFL behavior can be seen. Our main purpose is to identify this condition analyzing temperature dependence of the entropy by the NRG method and it will be emphasized that crossover from the NFL to FL regime can occur even if $|J_1 - J_2| > T_{\rm K}$.

The two-impurity Kondo model is also known to have a NFL critical point, which arises from competition between the interimpurity antiferromagnetic interaction and single-channel Kondo effects.[3] The nature of criticality of this system has been well understood.[3,23–26] The residual entropy is $\ln\sqrt{2}$ at the critical point just like the $n = 2$, $S = 1/2$ single impurity Kondo model which was discussed in the above. The staggered impurity susceptibility $\chi_{\rm s}$ is $\sim |\ln T|$ when $T_{\rm x} \ll T \ll T_{\rm K}$. Recently, it has been shown that a similar mechanism works in the model with the competition between the Kondo singlet and f^2-crystalline-electric-field singlet explaining the NFL behavior observed in $\rm R_{1-x}U_xRu_2Si_2$ (R=Th, Y and La, $x \leq 0.07$).[27,28]

The crossover temperature $T_{\rm x}$ of the two-impurity Kondo model is known to be proportinal to $(K_{\rm c} - K)^2$ where K is the interimpurity antiferromagnetic (RKKY) coupling constant and $K_{\rm c}$ is the critical coupling.[26] We will also elucidate an explicit expression of the crossover temperature of this model and discuss similarities of the crossover behavior to that of the two-channel anisotropic Kondo model in a magnetic field.

The organization of this paper is as follows. In §2, we discuss effects of channel anisotropy and a magnetic field in the two-channel Kondo model. In §3, we study the crossover behavior of the two-impurity Kondo model around the criticality. Finally, we summarize our results in §4.

§2. Anisotropic Two-Channel Kondo Model in a Magnetic Field

2.1 Model and numerical procedure

In this section, we discuss crossover from the NFL to FL regime in the $n = 2$, $S = 1/2$ Kondo model with channel anisotropy and in a magnetic field described by the following Hamiltonian:

$$H = H_{\rm K} + H_{\rm I} + H_{\rm Z}, \tag{2.1}$$

$$H_{\rm K} = \sum_{m=1,2} \sum_{k,\sigma} \epsilon_k c^\dagger_{km\sigma} c_{km\sigma}, \tag{2.2}$$

$$H_{\rm I} = \sum_{m=1,2} \sum_{k,k',\sigma,\sigma'} J_m c^\dagger_{km\sigma} \vec{\sigma}_{\sigma\sigma'} c_{k'm\sigma'} \cdot \vec{S}, \tag{2.3}$$

$$H_{\rm Z} = -2hS_z. \tag{2.4}$$

Here m $(= 1, 2)$ is the index of two channels, σ is the spin index, $c^\dagger_{km\sigma}$ is the creation operator of the conduction electron, $\vec{S}$ is the impurity spin and $\vec{\sigma}$ is the vector formed by the Pauli matrices. $H_{\rm Z}$ represents the Zeeman term where the g-factor is taken as 2. When $J_1{=}J_2$ and $h{=}0$, one obtains the isotropic two-channel Kondo Hamiltonian leading to the NFL stable fixed point. The case of $J_1{\neq}J_2$ corresponds to the anisotropic two-channel Kondo Hamiltonian whose stable fixed point is that of FL.

To analyze the Hamiltonian eq. (2.1) by the NRG method,[6–8] we transform eqs. (2.2) and (2.3) into

$$H_{\rm K} = \frac{(1+\Lambda^{-1})D}{2} \sum_{m=1,2} \sum_{n=0}^{\infty} \sum_{\sigma} \Lambda^{-n/2} \times (f^\dagger_{m,n\sigma} f_{m,n+1\sigma} + f^\dagger_{m,n+1\sigma} f_{m,n\sigma}), \tag{2.5}$$

$$H_{\rm I} = \frac{(1+\Lambda^{-1})D}{2} \sum_{m=1,2} \sum_{\sigma,\sigma'} J_m f^\dagger_{m,0\sigma} \vec{\sigma}_{\sigma\sigma'} f_{m,0\sigma'} \cdot \vec{S}, \tag{2.6}$$

where $f_{m,n}$ $(f^\dagger_{m,n})$ is annihilation (creation) operator of the conduction electron in the Wannier representation whose extent $k_{\rm F}^{-1}\Lambda^{n/2}$. Λ is a logarithmic discretization parameter in NRG calculation, D is half the bandwidth of the conduction electrons. Following an usual procedure of the NRG method, we define H_N as

$$H_N = \Lambda^{(N-1)/2} \Big[\sum_m \sum_\sigma \sum_{n=0}^{N-1} \Lambda^{-n/2} (f^\dagger_{m,n\sigma} f_{m,n+1\sigma} + \text{h.c}) + J_m \sum_{\sigma,\sigma'} f^\dagger_{m,0\sigma} \vec{\sigma}_{\sigma,\sigma'} f_{m,0\sigma'} \cdot \vec{S} \Big]. \tag{2.7}$$

Then, the Hamiltonian (2.7) satisfies the recursion relation

$$H_{N+1} = \Lambda^{1/2} H_N + \sum_{m,\sigma} (f^\dagger_{m,N\sigma} f_{m,N+1\sigma} + f^\dagger_{m,N+1\sigma} f_{m,N\sigma}). \tag{2.8}$$

By repeated use of the recursive procedure, we can compute the eigen states and energy levels of Hamiltonians (H_N).

Once the energy levels of H_N are obtained, the entropy can be calculated by the relation

$$S = \beta_N(\langle H_N \rangle - F_N), \tag{2.9}$$

in each N-step. Here $\langle H_N \rangle$ and F_N are defined as

$$\begin{aligned} \langle H_{\rm N} \rangle &= \frac{{\rm Tr} H_N e^{-\beta_N H_N}}{{\rm Tr} e^{-\beta_N H_N}}, \\ F_N &= -\frac{1}{\beta_N} \ln Z_N = -\frac{1}{\beta_N} \ln({\rm Tr} e^{-\beta_N H_N}), \end{aligned} \tag{2.10}$$

where $\beta_N = \Lambda^{-(N-1)/2}/T$. By setting $T \sim T_N \equiv \Lambda^{-(N-1)/2}$, we can obtain temperature dependence of the entropy with a good accuracy in NRG calculation.

In our calculation, we set $\beta_N^{-1} = 0.5$ and $\Lambda = 3$ and about 600 total states are retained at each iteration. Hereafter, we take the unit of energy as $(1 + \Lambda^{-1})D/2$.

2.2 Crossover temperature $T_{\rm x}$

In this subsection, we elucidate an explicit expression of the crossover temperature $T_{\rm x}$ of the model, eq. (2.1), from NRG results on the impurity entropy $S_{\rm imp}(T)$. As mentioned in §1, if $0<T_{\rm x}/T_{\rm K}\ll 1$, $S_{\rm imp}(T)$ of this model decreases from $1/2 \cdot \ln 2$ to 0 around $T_{\rm x}$ as T is lowered. So $T_{\rm x}$ can be defined as temperature at which the entropy takes a value of $S_{\rm imp}(T_{\rm x})=1/4 \cdot \ln 2$, the middle point between NFL and FL fixed points. (For examples, see Fig. 2 below.)

Firstly, we investigate an effect of channel anisotropy on $T_{\rm x}$ for $h = 0$. In this case, we can assume that $T_{\rm x}$ is described by a function of two parameters, i.e., $J_{\rm av} \equiv (J_1 + J_2)/2$ and $\Delta J \equiv J_1 - J_2$. Our procedure to determine $T_{\rm x}$ is illustrated in Fig. 2 (a) and (b) which present NRG results on $S_{\rm imp}(T)$ for $J_{\rm av} = 0.1$, $\Delta J = 1.0 \times 10^{-4}$ and for $J_{\rm av} = 10$, $\Delta J = 1.0 \times 10^{-3}$, respectively. It is noted that $T_{\rm x}/T_{\rm K} \ll 1$ while $\Delta J \gtrsim T_{\rm K}$ in both (a) and (b). These examples lead us to the fact that $T_{\rm x}$ is not scaled as $T_{\rm x} \sim \Delta J^2/T_{\rm K}$. (If $T_{\rm x}$ were $\sim \Delta J^2/T_{\rm K}$, ΔJ should be much less than $T_{\rm K}$ for $T_{\rm x}/T_{\rm K} \ll 1$.) Actually, we have tested a bunch of parameter sets and found a function which reproduces the behavior of $T_{\rm x}$ as follows:

$$T_{\rm x} = \alpha \times (\Delta \tilde{J}/\tilde{J}_{\rm av})^2 e^{-1/\tilde{J}_{\rm av}}, \tag{2.11}$$

where α is a numerical constant which is taken to be $\alpha = 2.95$ within the accuracy of our calculation, and

$$\Delta \tilde{J} = A_\Lambda \Delta J, \tag{2.12}$$

$$\tilde{J}_{\rm av} = A_\Lambda J_{\rm av}, \tag{2.13}$$

$$A_\Lambda = \frac{1}{2}\frac{1 + \Lambda^{-1}}{1 - \Lambda^{-1}} \ln \Lambda. \tag{2.14}$$

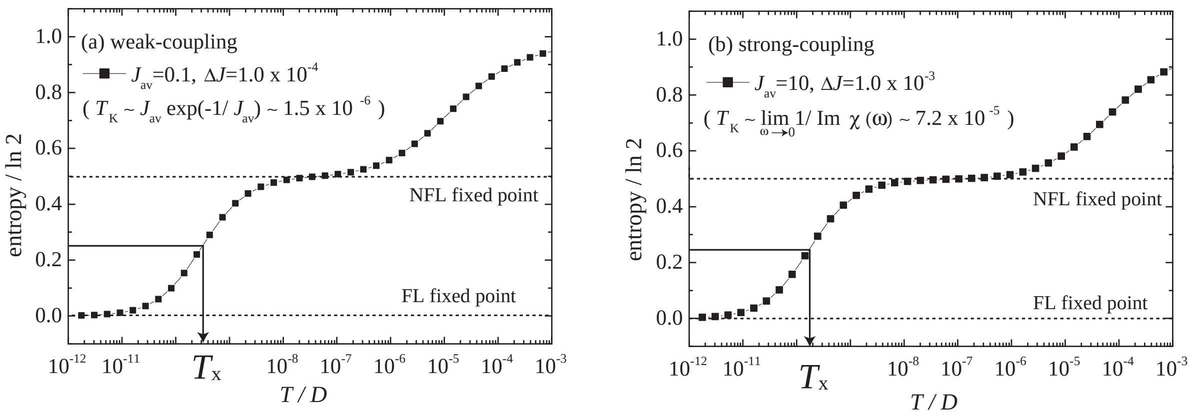

Fig. 2. NRG results on the entropy $S_{\rm imp}(T)$ of the anisotopic two-channel Kondo model for (a) $J_{\rm av}=0.1$, $\Delta J=1.0\times10^{-4}$ and for (b) $J_{\rm av}=10$, $\Delta J=1.0\times10^{-3}$. In each case, crossover from NFL to FL regime can be clearly seen, i.e. $T_{\rm x}/T_{\rm K}\ll1$, and then $T_{\rm x}$ is obtained by the relation $S_{\rm imp}(T_{\rm x})=1/4\cdot\ln2$.

Here A_Λ is a revision factor of the density of states in NRG calculation. Fig. 3 shows that $T_{\rm x}$ is well fitted by eq. (2.11). From Fig. 3 (a) in which $J_{\rm av}$=0.3 is fixed, $T_{\rm x}$ can be seen to be proportional to ΔJ^2, which is consistent with the results of Pang and Cox.[16] On the other hand, from Fig. 3 (b) in which ΔJ=1.0×10^{-3} is fixed, $J_{\rm av}$-dependence of $T_{\rm x}$ can be seen to be equivalent to that of the right hand side of eq. (2.11). In the weak-coupling case of $J_{\rm av}\lesssim0.4$, $T_{\rm x}$ is an increasing function of $J_{\rm av}$ as can be seen in Fig. 3 (b) while $T_{\rm K}$ is well known to be an increasing function $\sim J_{\rm av}e^{-1/J_{\rm av}}$ in the case of $n=2$ by the two-loop perturbative renormalization group theory. It is noted that if $T_{\rm x}$ were $\sim\Delta J^2/T_{\rm K}$, $T_{\rm x}$ should be a decreasing function of $J_{\rm av}$ in the weak-coupling regime. (See also Fig. 4 (b) for comparison.)

We have checked that eq. (2.11) can be adopted in a wide parameter region of $J_{\rm av}$ for the $n=2$, $S=1/2$ Kondo model with channel anisotropy. In the weak-coupling regime, from eq. (2.11) and $T_{\rm K}\sim J_{\rm av}e^{-1/J_{\rm av}}$, the condition that crossover from NFL to FL regime occurs, i.e. $T_{\rm x}/T_{\rm K}\ll1$, is given explicitly by $\Delta J^2/J_{\rm av}^3\ll1$. This result indicates that the NFL behavior in the two-channel Kondo model is fairly robust against channel anisotropy.

Next, we investigate an effect of a magnetic field in the isotropic channel case of J_1=$J_2$$\equiv$$J$. In this case, as mentioned in §1, $T_{\rm x}$ is $\sim h^2/T_{\rm K}$.[9,15,17] As shown in Fig. 4 (a) and (b), it can be actually

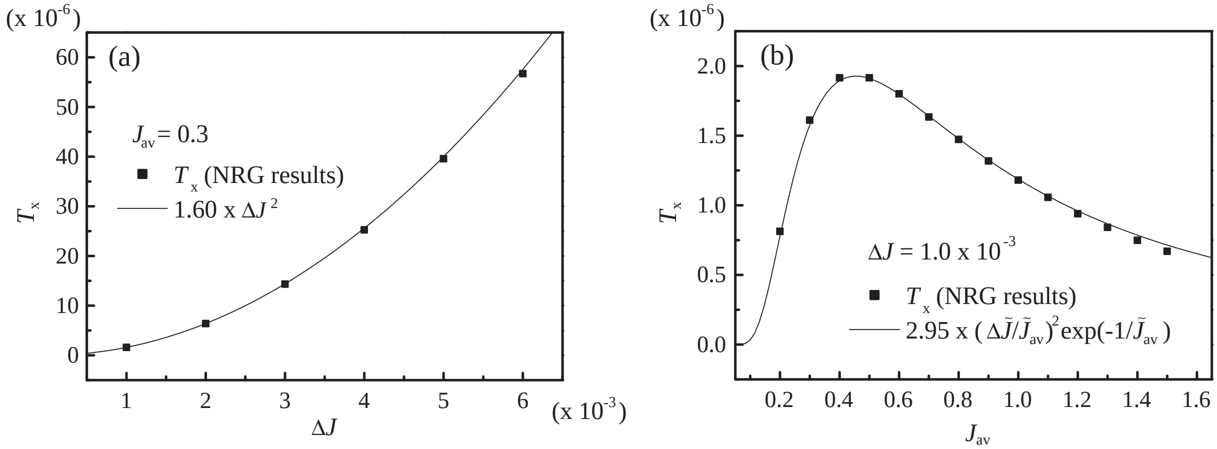

Fig. 3. Crossover temperature (T_{x}) of the two-channel Kondo model with channel anisotropy (ΔJ). (a) T_{x} versus ΔJ with J_{av}=0.3 fixed. (b) T_{x} versus J_{av} with ΔJ=1.0 $\times$ 10^{-3} fixed. T_{x} is well fitted by eq.(2.11).

checked from our NRG results on the entropy that T_{x} can be well fitted by a function of

$$T_{\mathrm{x}} = \beta \times h^2/T_{\mathrm{K}}, \tag{2.15}$$

where β is a numerical constant of $\beta = 4.45$. Here T_{K} is defined in terms of the dynamical impurity susceptibility $\chi(\omega)$ by

$$T_{\mathrm{K}} \propto \lim_{\omega \to 0} \lim_{T \to 0} \left[\mathrm{Im}\chi(\omega)\right]^{-1}, \tag{2.16}$$

for the isotropic channel model in the absence of a magnetic field[29–31] in which the value of T_{K} is normalized to coincide with $Je^{-1/J}$ ($\equiv T_{\mathrm{K}}^{p}$) at J=0.1. Eq. (2.15) is valid in a wide region from weak to strong coupling. This suggests that eq. (2.16) is a good definition of T_{K}. In Fig. 5, we show J-dependence of T_{K}, which is defined by eq. (2.16), and of T_{K}^{p}, which is the two-loop perturbative renormalization group result. While T_{K}^{p} is a monotonously increasing function of J, T_{K} exhibits a broad peak at or around $J{\sim}1.3$. The discrepancy between T_{K} and T_{K}^{p} indicates that the two-loop perturbative renormalization group result on the Kondo temperature is not sufficient for $J \gtrsim 0.5$.

2.3 Scaling function for entropy in the crossover regime

We have obtained an explicit expression of T_{x}, eq. (2.11), in the conventional band-width cutoff scheme for the $n = 2$, $S = 1/2$ Kondo model with channel anisotropy. On the other hand, the thermodynamic Bethe ansatz (TBA) equations for the anisotropic multichannel Kondo model was obtained by Andrei and Jerez.[21] While their cutoff scheme differs substantially from ours, and so

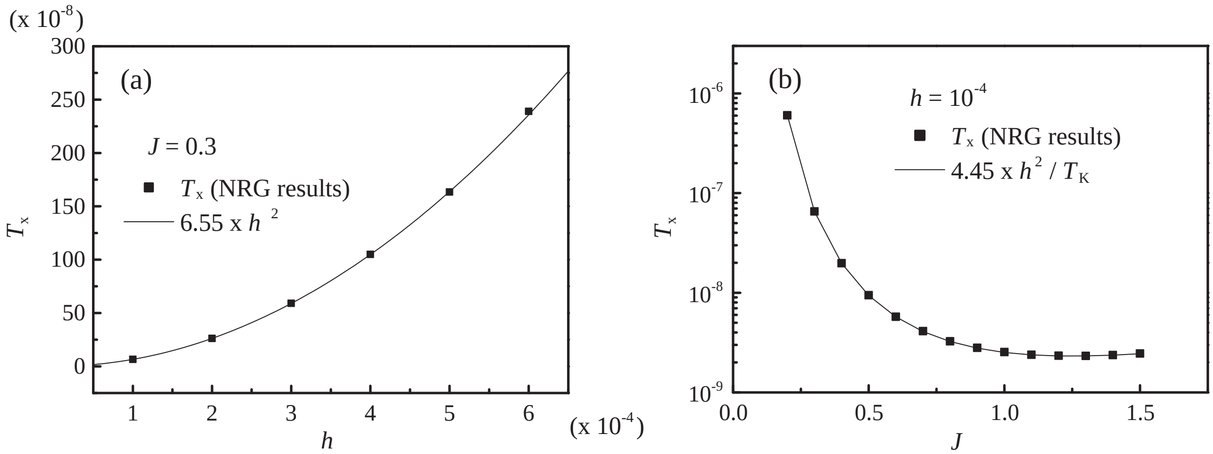

Fig. 4. Crossover temperature ($T_{\rm x}$) of the two-channel Kondo model in the presense of a magnetic field (h). (a) $T_{\rm x}$ versus h with J=0.3 fixed. (b) $T_{\rm x}$ versus J with h=1.0 $\times$ 10^{-4} fixed. $T_{\rm x}$ is well fitted by eq. (2.15).

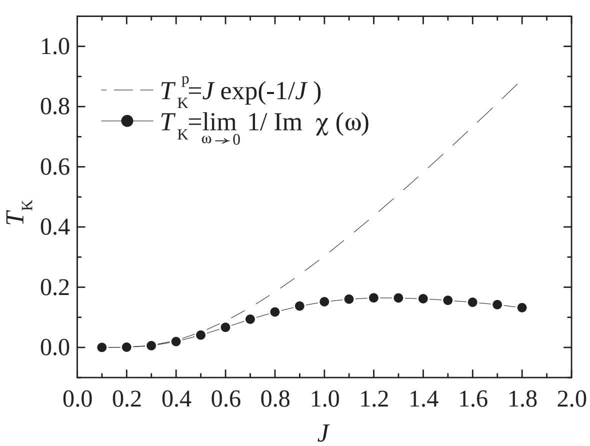

Fig. 5. J-dependence of $T_{\rm K}$ defined by eq. (2.16) compared with $T_{\rm K}^{p}$=$Je^{-1/J}$.

does their expression of $T_{\rm x}$ ($T_{\rm K}$), their $n = 2$, $S = 1/2$ model must be in the same universality class as ours. It is thus possible to make a comparison of our NRG results with the TBA result by use of our expression of $T_{\rm x}$ (if necessary, $T_{\rm K}$). In this subsection, we concentrate on the crossover regime

in which $0 \lesssim S_{\rm imp}(T) \lesssim \ln\sqrt{2}$, $T \ll T_{\rm K}$, and explicitly show that our NRG results on the entropy can be fitted by a scaling function of $T/T_{\rm x}$.

First, we derive the scaling function in the crossover regime analytically from the TBA equations. In the scaling limit, the impurity part of the free energy is given by[21)]

$$F_{\rm imp}(T) = -\frac{T}{2\pi}\int_{-\infty}^{\infty}\frac{\ln[1+\eta_1(\xi)]}{\cosh[\xi+\ln(T/T_{\rm K})]}{\rm d}\xi, \tag{2.17}$$

where $\eta_1(\xi)$ is determined by the TBA equations;

$$\ln\eta_1(\xi) = -2r{\rm e}^{\xi} + G*\ln[1+\eta_2(\xi)], \tag{2.18}$$

$$\ln\eta_2(\xi) = -{\rm e}^{\xi} + G*\ln[1+\eta_1(\xi)] + G*\ln[1+\eta_3(\xi)], \tag{2.19}$$

$$\ln\eta_j(\xi) = G*\ln[1+\eta_{j-1}(\xi)] + G*\ln[1+\eta_{j+1}(\xi)], \quad j\geq 3, \tag{2.20}$$

with a boundary condition

$$\lim_{j\to\infty}\frac{\ln\eta_j(\xi)}{j} = \frac{2h}{T}. \tag{2.21}$$

Here $G*\varphi(\xi)\equiv\int_{-\infty}^{\infty}G(\xi-\xi')\varphi(\xi'){\rm d}\xi'$ and $G(\xi-\xi')\equiv 1/2\pi\cosh(\xi-\xi')$. For $T\ll T_{\rm K}$, the impurity free energy, eq. (2.17), is determined by the $\xi\to+\infty$ asymptotic form of η_1. In the limit of $\xi\to+\infty$, η_j is given by

$$\eta_j(+\infty) = \frac{\sinh^2[(j-1)h/T]}{\sinh^2(h/T)} - 1, \quad j\geq 2. \tag{2.22}$$

Firstly, we consider the case of $T\ll h\ll T_{\rm K}$. By eq. (2.22), $\eta_3(+\infty)\simeq\exp(2h/T)$ and its corrections due to ξ dependence can be neglected, so that eq. (2.19) leads to

$$\ln\eta_2(\xi) = -{\rm e}^{\xi} + h/T + f(r,{\rm e}^{-\xi},h/T), \tag{2.23}$$

where f is defined by eq. (1.2). In eq. (2.23), the last term can be seen to compare negligibly with h/T if we note that this term is $\sim F_{\rm imp}(T)/T$ in a region around $\xi\sim\ln(T_{\rm K}/T)$. Then, after some manipulations of eqs. (2.17), (2.18) and (2.23), we obtain

$$F_{\rm imp}(T) \sim -\frac{T}{2\pi}\int_{-\infty}^{\infty}\frac{\ln[1+\exp(-(h/T)\varepsilon(\zeta))]}{\cosh[\zeta+\ln(h/T_{\rm K})]}{\rm d}\zeta, \tag{2.24}$$

where $\varepsilon(\zeta)$ is given by

$$\varepsilon(\zeta) = {\rm e}^{\zeta}\left(2r+\frac{1}{2\pi}\ln\left(1+{\rm e}^{-2\zeta}\right)-\frac{1}{\pi}{\rm e}^{-\zeta}\tan^{-1}\left({\rm e}^{-\zeta}\right)\right), \tag{2.25}$$

$$\sim {\rm e}^{\zeta}\left(2r-{\rm e}^{-2\zeta}/2\pi\right), \qquad \text{for} \quad {\rm e}^{-\zeta}\sim h/T_{\rm K}\ll 1. \tag{2.26}$$

The integral in eq. (2.24) has dominant contributions from a region around $\zeta\sim\ln(T_{\rm K}/h)$. When $r\gg(h/T_{\rm K})^2$, the second term can be neglected in eq. (2.26) so that the impurity free energy can

be written in the following scaling form:

$$F_{\text{imp}}(T) = -T\tilde{f}(T/T_{\text{x}}), \tag{2.27}$$

where the crossove temperature is given by $T_{\text{x}} = rT_{\text{K}}$ and $\tilde{f}$ is a scaling function in the crossover regime;

$$\tilde{f}(x) = \int_{-\infty}^{\infty} \frac{\ln[1+\exp(-2\exp(\xi))]}{2\pi\cosh[\xi+\ln(x)]}\mathrm{d}\xi \tag{2.28}$$

$$= \frac{1}{\pi x}\ln\frac{1}{\pi x} - \frac{1}{\pi x} - \ln\Gamma\left(\frac{1}{\pi x}+\frac{1}{2}\right) + \frac{1}{2}\ln 2\pi, \tag{2.29}$$

where Γ is the gamma function. Then, the impurity entropy, $S_{\text{imp}}{=}-\partial F_{\text{imp}}/\partial T$, is calculated as

$$S_{\text{imp}}(T) = \frac{1}{\pi(T/T_{\text{x}})}\psi\left(\frac{1}{\pi(T/T_{\text{x}})}+\frac{1}{2}\right) - \frac{1}{\pi(T/T_{\text{x}})} - \ln\Gamma\left(\frac{1}{\pi(T/T_{\text{x}})}+\frac{1}{2}\right) + \frac{1}{2}\ln 2\pi, \tag{2.30}$$

where ψ is the digamma function. On the other hand, when $r \ll (h/T_{\text{K}})^2$, the first term can be neglected in eq.(2.26). In this case, if the crossover temperature is regarded as $T_{\text{x}}{=}h^2/4\pi T_{\text{K}}$, T-dependent contributions in the impurity free energy is given by $-T\tilde{f}(T/T_{\text{x}})$ and therefore eq. (2.30) is also available for the entropy.

Secondly, we consider the case of $h{\lesssim}T{\ll}T_{\text{K}}$. By eqs. (2.19) and (2.22), $\ln\eta_2(\xi){\simeq}-\mathrm{e}^{-\xi}$ so that $\ln\eta_1(\xi){\simeq}-2r\mathrm{e}^{\xi}$. Hence eq. (2.30) is available by $T_{\text{x}}{=}rT_{\text{K}}$. It is noted that if $r \ll (h/T_{\text{K}})^2$, $T_{\text{x}}{=}rT_{\text{K}}{\ll}h{\lesssim}T$ so that the entropy is $\sim\ln\sqrt{2}$, which is not sensitive to the value of T_{x}.

In summary, a scaling function for entropy in the crossover regime is given by eq. (2.30) where $T_{\text{x}}{=}rT_{\text{K}}$ for $r{\gg}(h/T_{\text{K}})^2$ and $T_{\text{x}}{=}h^2/4\pi T_{\text{K}}$ for $r{\ll}(h/T_{\text{K}})^2$. For eq. (2.30), $S_{\text{imp}}(T_{\text{x}}){=}0.99{\times}1/4{\cdot}\ln 2$ so that T_{x} is about the same as we defined in the former subsection. (We must apologize for the normalization schemes on T_{K} which are different between the former and this subsections.)

Second, we compare our NRG results on entropy with eq. (2.30). Figures 6 and 7 present the results on entropy versus temperature scaled by T_{x}, expressions of which are eq. (2.11) and eq. (2.15), in the anisotropic channel case and in the presence of a magnetic field, respectively. In both cases, the T dependence of entropy can be fitted quite well in the crossover regime by the scaling function, eq. (2.30), derived from the TBA equations.

§3. Two-Impurity Kondo Model

3.1 Model

In this section, we study the two-impurity Kondo model whose Hamiltonian is given by two independent Kondo models coupled by interimpurity exchange interaction (K) as follows:

$$H = H_{\text{K}} + H_{\text{I}}' + H_{\text{L}}, \tag{3.1}$$

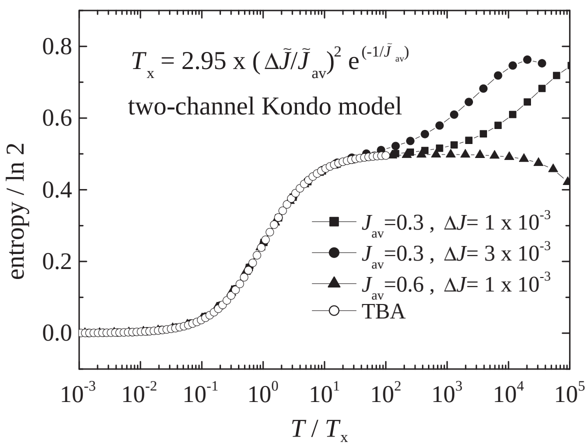

Fig. 6. Temperature dependences of entropy obtained by the NRG method for the anisotropic two-channel Kondo model. In the crossover regime, by use of an expression of T_{x}, eq. (2.11), they can be fitted quite well by a scaling function, eq. (2.30) derived from the TBA equations.

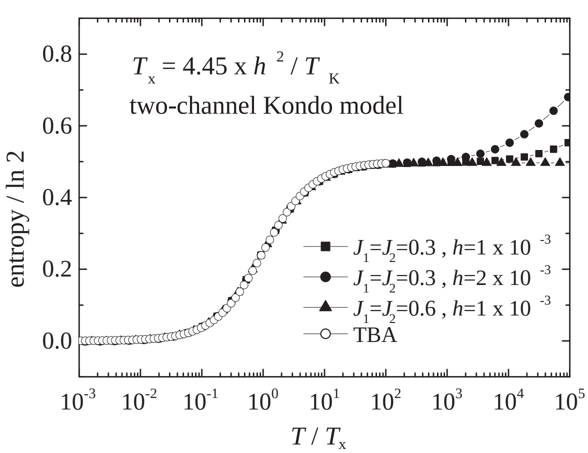

Fig. 7. Temperature dependence of entropy obtained by the NRG method for the two-cannel Kondo model in the presence of a magnetic field. In the crossover regime, by use of an expression of T_{x}, eq. (2.15), they can be fitted quite well by a scaling function, eq. (2.30) derived from the TBA equations.

$$H_{\mathrm{K}} = \sum_{m=1,2} \sum_{k,\sigma} \epsilon_k c^{\dagger}_{km\sigma} c_{km\sigma}, \tag{3.2}$$

$$H'_{\mathrm{I}} = \sum_{m=1,2} J_m \sum_{k,k',\sigma,\sigma'} c^{\dagger}_{km\sigma} \vec{\sigma}_{\sigma\sigma'} c_{k'm\sigma'} \cdot \vec{S}_m, \tag{3.3}$$

$$H_{\mathrm{L}} = K \vec{S}_1 \cdot \vec{S}_2. \tag{3.4}$$

The notations are the same as before. In the original form of the two-impurity Kondo model studied by Jones *et al.*,[3] the Kondo exchange coupling between the conduction electrons and localized spin with both the same and different symmetry (specified by m) are taken into account, because they considered the case of the two impurities on different sites. In the present study, we neglect the Kondo exchange coupling between different symmetries, for simplicity. It is however noted that our model, eq. (3.1), itself can be considered to be a local-moment version of the two-orbital Anderson model with crystalline-electric-field (CEF) effect in a certain pseudospin representation.[27,28]

The model, eq. (3.1) has a NFL fixed point at $K{=}K_{\mathrm{c}}(J_1, J_2)$ for a set of J_1 and J_2 due to competition between the single channel Kondo effects and the interimpurity antiferromagnetic interaction.[3,23–28,32] In this section, we concentrate on the region around critical points of $K{=}K_{\mathrm{c}}(J, J)$. The definition of T_{x} is the same as that of the former section; $S_{\mathrm{imp}}(T_{\mathrm{x}}){=}1/4 \cdot \ln 2$.

3.2 Crossover temperature T_{x} *in the region around critical points of* $K{=}K_{\mathrm{c}}(J, J)$

Firstly, we consider cases in which K is displaced slightly away from a critical value of $K_{\mathrm{c}}{\equiv}K_{\mathrm{c}}(J, J)$ with $J_1{=}J_2{=}J$ fixed. It has already been discussed by using the conformal field theory that T_{x} is proportional to $\Delta K^2/T_{\mathrm{K}}$,[26] where $\Delta K{=}K_{\mathrm{c}} - K$. Here we define T_{K} by

$$T_{\mathrm{K}} \equiv \lim_{\omega\to 0} \lim_{T\to 0} 1/\mathrm{Im}\chi_{\mathrm{s}}(\omega), \tag{3.5}$$

where χ_{s} is the dynamical impurity susceptibility for $\vec{S}_1 - \vec{S}_2$. We have examined various parameter sets and confirmed that the crossover temperature T_{x} is given as

$$T_{\mathrm{x}} = \gamma \times \Delta K^2/T_{\mathrm{K}}, \tag{3.6}$$

where γ is a numerical constant of $\gamma{=}0.50$ within the accuracy of our calculation. In fact, as shown in Fig. 8, the temperature dependence of entropy can be scaled by T_{x} defined by eq.(3.6) quite well.

Next, we consider cases in which J_2 is displaced slightly away from $J_2{=}J$ with $J_1{=}J$ and $K{=}K_{\mathrm{c}}{\equiv}K_{\mathrm{c}}(J, J)$ fixed. In Fig. 9, we show the behavior of a crossover for $J_1{=}0.3$, $J_2{=}0.297$, and $K{=}K_{\mathrm{c}}{=}0.195416$, compared with the case of the two-channel Kondo model with $J_1{=}0.3$ and $J_2{=}0.297$. The isotropic channel cases in both models are also shown in this figure. In both cases, the small perturbation $(J_1 - J_2)$ does not affect the high temperature behavior. Namely, it does not change T_{K}. The temperature dependence of entropy in the anisotropic channel case is quite similar in both cases in the crossover regime. Hence T_{x} for the two-impurity model is also given by eq. (2.11).

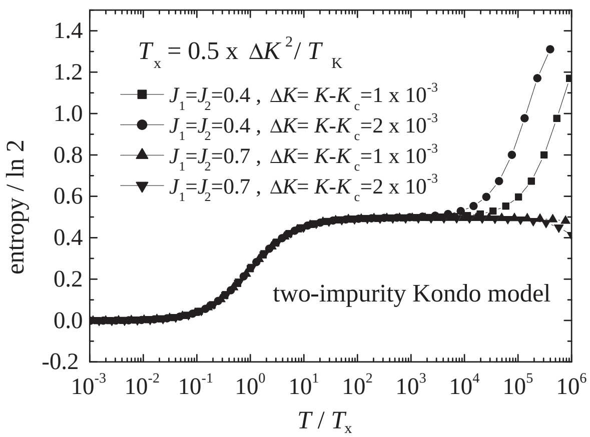

Fig. 8. Temperature dependence of entropy for the two-impurity Kondo model when K is displaced slightly away from K_c. K_c=0.564723 for J_1=J_2=0.4. K_c=2.655538 for J_1=J_2=0.7. The temperature is scaled by T_x, which is determined by eqs. (3.5) and (3.6).

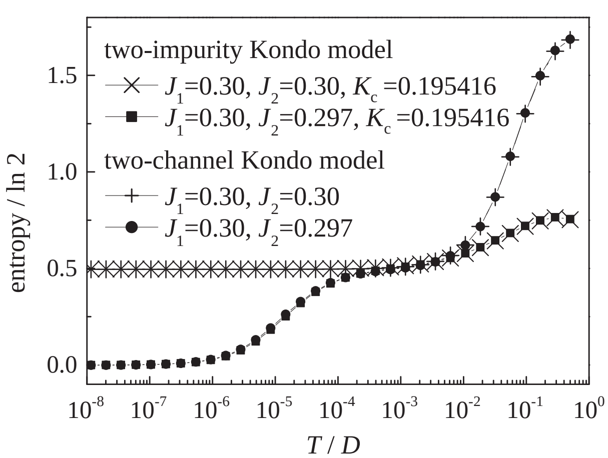

Fig. 9. Crossover behavior for the two-impurity Kondo model (J_1=0.3, J_2=0.297, and K=K_c=0.195416), compared with the case of the anisotropic two-channel Kondo model with J_1=0.3 and J_2=0.297.

§4. Summary

In this paper, we have investigated effects of relevant perturbations, which bring about crossover from the NFL to FL regime, in the regions around quantum critical points of the two-channel and two-impurity Kondo models.

For the two-channel Kondo model in which $T_{\rm K}$ is defined by $T_{\rm K} \propto \lim_{\omega\to 0} \lim_{T\to 0}[{\rm Im}\chi(\omega)]^{-1}$ (in the weak-coupling regime, $T_{\rm K}{\simeq}J_{\rm av}{\rm e}^{-1/J_{\rm av}}$), we have derived numerically exact expressions of the crossover temperature $T_{\rm x}$ from our NRG results on the entropy as follows: (1) in the anisotropic channel case, if $T_{\rm x}/T_{\rm K}{\ll}1$ (in the weak-coupling regime, $\Delta J^2/J_{\rm av}^3{\ll}1$), crossover from the NFL to FL regime occurs around $T_{\rm x}$ which is given by $T_{\rm x}{=}\alpha{\times}(\Delta\tilde{J}/\tilde{J}_{\rm av})^2 e^{-1/\tilde{J}_{\rm av}}$ with α=2.95, where $J_{\rm av}$ and ΔJ are the average and difference of the exchange couplings J_1 and J_2, respectively (a swung dash means A_Λ times, A_Λ being a revision factor of the order of 1); (2) in the presence of a magnetic field, if $(h/T_{\rm K})^2{\ll}1$, crossover from the NFL to FL regime occurs around $T_{\rm x}$ which is given by $T_{\rm x}{=}\beta \times h^2/T_{\rm K}$, where β=4.45 in our normalization procedure on $T_{\rm K}$.

For the two-impurity Kondo model which has a NFL critical point at $K{=}K_{\rm c}(J_1, J_2)$ for a set of the Kondo exchange couplings J_1 and J_2, we have obtained NRG results on the entropy in the region around critical points of $K{=}K_{\rm c}(J, J)$ as follows: (1) when J_2 is displaced slightly away from $J_2{=}J$ with $J_1{=}J$ and $K{=}K_{\rm c}(J, J)$ fixed, crossover to a FL fixed point occurs around $T_{\rm x}$ which is given by that of the two-channel Kondo model with the same set of J_1 and J_2 in the absence of a magnetic field; (2) when interimpurity (RKKY) exchange coupling K is displaced slightly away from the critical value of $K_{\rm c}(J, J)$ with $J_1{=}J_2{=}J$ fixed, crossover to a FL fixed point occurs around $T_{\rm x}$ which is given by $T_{\rm x}{=}\gamma \times (K_{\rm c} - K)^2/T_{\rm K}$ with γ=0.50 where $T_{\rm K}{\equiv}\lim_{\omega\to 0}\lim_{T\to 0}\ {\rm Im}\chi_{\rm s}(\omega)$.

In the present work, all the results on $T_{\rm x}$ can be adopted in a wide region of J ($J_{\rm av}$) and all the temperature dependences of entropy in the crossover regime can be fitted quite well by a scaling function, eq. (2.30), derived from the TBA equations of the two-channel Kondo model with channel anisotropy and in the presence of a magnetic field. It is emphasized that the NFL behavior in the two channel Kondo model is fairly robust against channel anisotropy so that crossover from the NFL to FL regime can be seen even if $\Delta J{>}T_{\rm K}$.

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